DATA QUALITY SUMMARY REPORT FOR SULFUR DIOXIDE DATA COLLECTED BY SONOMA TECHNOLOGY, INC., DURING THE CALIFORNIA REGIONAL $PM_{10}/PM_{2.5}$ AIR QUALITY STUDY

By:
Nicole P. Hyslop
Steven G. Brown
Courtney A. Gorin
Hilary R. Hafner
Sonoma Technology, Inc.
1360 Redwood Way, Suite C
Petaluma, CA 94954-1169

Prepared for:
San Joaquin Valleywide Air Pollution Study Agency
c/o Karen Magliano
California Air Resources Board
1001 "I" Street
Sacramento, California 95814

February 20, 2003

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1. INTRODUCTION AND OBJECTIVES

The purpose of this Data Quality Summary Report is to provide data users with an understanding of the quality of sulfur dioxide (SO_2) data collected by Sonoma Technology, Inc. (STI) for the California Regional $PM_{10}/PM_{2.5}$ Air Quality Study (CRPAQS). **Table C-1** lists the operating dates and sites for SO_2 concentration measurements during CRPAQS. This report provides summary information on data completeness, lower quantifiable limit (LQL), accuracy, and precision. SO_2 concentrations were measured with 1-minute time resolution and averaged to 5-minute and 60-minute values. Only the 5-minutes and 60-minute data were reported. Data completeness, based on data delivered to ARB, and LQL were calculated for both 5-minute and 60-minute data while accuracy and precision were calculated using nightly calibration data and are applicable to both 5-minute and 60-minute data. Start date/time indicates the beginning of valid data, continuous until the stop date/time. Only one SO_2 monitor was operated by STI.

Table C-1. Location and duration of SO_2 measurements made by STI during CRPAQS.

Site	Start Date/Time	Stop Date/Time
Bakersfield	11/20/00 19:30 PST	2/8/01 23:55 PST

Several other documents are available from which to obtain information about the CRPAQS field study and data processing. Sampling locations are described in Wittig et al. (2003). Quality control screening procedures are summarized by Hafner et al. (2003). Results of systems and performance audits and intercomparisons are provided by Bush et al. (2001).

The data quality objectives (DQOs) for SO_2, in accordance with the CRPAQS Quality Integrated Work Plan (QIWP), (1999) are shown in **Table C-2**. All Bakersfield data met the CRPAQS DQO criteria.

Table C-2. Data quality objectives for SO_2 data collected during CRPAQS.

Data Quality Metric	CRPAQS Objective
Completeness	90%
Lower Quantifiable Limit	0.2 ppb
Accuracy	0.2 ppb or 95% Confidence Interval ≤ 10%
Precision	0.2 ppb

2. DATA COMPLETENESS

Data completeness for all SO_2 measurement sites for both 5-minute and 60-minute data is detailed in **Table C-3**. Data capture quantifies the percentage of total records received versus the

number expected during the "period of operation" defined by the start and stop dates/times in Table C-1; the start date/time is the first instance of valid data, and the period of operation is continuous until the stop date/time. The number of valid data points is divided by the number of captured data points to calculate the data recovery. Validity is defined for this calculation as any data point that has a quality control flag of V0 (valid) or V1 (valid but comprised wholly or partially of below-MDL data). Details of data validation are included in Hafner et al. (2003).

Table C-3. SO_2 data completeness values for the Bakersfield site.

Monitoring Site	No. of Total Records	Expected No. of Records	Percent Capture[a.]	No. of Valid Records	Percent Recovery[b]	No. of Suspect Records	No. of Invalid Records	No. of Missing Records
Bakersfield (5-min)	23,094	23,094	100%	22,043	95%	17	1031	3
Bakersfield (60-min)	1925	1925	100%	1858	97%	0	67	0

[a.] % capture = total number of records/expected records*100
[b.] % recovery = number of valid records/total numbers of records

The data capture rate for SO_2 was 100%. The data recovery rate ranged from 95% (5-minute) to 97% (60-minute); these recovery rates meet the CRPAQS DQO.

3. LOWER QUANTIFIABLE LIMIT

The LQL is the lowest concentration in ambient air that can be measured when processing actual samples. Sources of variability that influence the monitored signal at low concentrations include instrument noise and atmospheric variability. As a measure of this variability, two times the standard deviation of selected 5-minute and 60-minute data was used to estimate the LQL. The selected data were collected during relatively stable periods with concentrations close to zero. This is a conservative estimate of the LQL because it includes the concentration variability of the ambient air. Twelve consecutive data values were used to compute the LQL with the 5-minute data and six data values with the 60-minute data; atmospheric variation generally becomes too great after six hours to calculate a reasonable LQL. Since only half the number of data values were used in the calculation (see "N" in Equation C-1), the 60-minute LQL is expected to be higher than the 5-minute LQL, despite the "smoothing" that occurs when averaging 5-minute to 60-minute values.

The LQL is calculated as shown in Equation C-1. **Table C-4** shows the LQL for the sampling period, as well as the specific data strings used to calculate the LQLs. The LQLs for both sampling intervals meet the CRPAQS DQO. For SO_2, the LQL for the 60-minute data was lower than the LQL for 5-minute data.

$$\text{LQL} \approx 2s = 2\sqrt{\frac{\sum (SO_2 - \overline{SO}_2)^2}{N-1}} \qquad \textbf{(C-1)}$$

where:

$\overline{SO_2}$ = mean SO_2 concentration
N = number of measurements
σ = standard deviation

Table C-4. Dates and times used to calculate SO_2 LQL, the LQL, and the corresponding mean concentration during the selected time period.

Type of Data	Dates and Times Used for LQL Calculation	LQL (ppb)	Mean (ppb)
5-minute	2/6/01 23:25 – 2/7/01 00:25 PST	0.14	0.01
60-minute	1/29/01 21:00 – 1/30/01 02:00 PST	0.08	0.04

4. ACCURACY

The accuracy of SO_2 measurements can be evaluated using the deviation of measurements from a standard reference. This method quantifies the variability in the routine accuracy of the instrument by evaluating the span checks, which were performed almost nightly in CRPAQS.

Span checks were performed at 40 ppb SO_2 using the on-site calibrator nearly every night. These nightly checks can be used to evaluate the accuracy of the instrument throughout the study. Accuracy can be expressed in terms of the 95% confidence interval (CI). For STI's SO_2 measurements, the 95% CIs were calculated from the differences between monitor response and known concentrations provided by the automatic span checks performed almost nightly during routine operation. The 95% CI approximates the accuracy of the data as shown in Equation C-2.

$$\text{Accuracy} \approx 95\%\ \text{confidence interval} = 1.96\left(\frac{s_{span}}{\sqrt{N}}\right) \qquad \textbf{(C-2)}$$

where:

$$s_{span} = \sqrt{\frac{\sum (x - \bar{x})^2}{N-1}}$$

$$x = [SO_2]_{cal} - [SO_2]_{measured}$$

$$\bar{x} = \frac{\sum ([SO_2]_{cal} - [SO_2]_{measured})}{N}$$

$[SO_2]_{cal}$ = SO_2 concentration output by the calibrator

$[SO_2]_{measured}$ = SO_2 concentration measured by the analyzer.

Generally, one 5-minute average of span check data was obtained. Only span checks at 40 ppb SO_2 were included. The 95% confidence intervals and the number of nightly average span values used to estimate the CI for SO_2 at Bakersfield are provided in **Table C-5**. The accuracy computed using span check data meets the CRPAQS DQO.

Table C-5. Accuracy at 40 ppb SO_2 and number of span check data points used for the 5-minute SO_2 concentrations at Bakersfield.

No. of Spans Used	Accuracy at 40 ppb SO_2
65	0.2 ppb

5. PRECISION

The consistency of the nightly span concentrations provides a measure of precision in the SO_2 analyzer measurements. The precision was evaluated by comparing the measured concentration during the span check to the average measured concentration during span checks for the entire study. Only span checks at 40 ppb SO_2 were included. The CI at a 95% confidence limit of the span measurements was used to estimate the precision of the data as shown in Equation C-3. This is applicable to both 5-minute and 60-minute data.

$$\text{Absolute Precision} \approx \text{CI} = 1.96 \times \frac{\sigma_{\text{measured}}}{\sqrt{N}} \qquad \textbf{(C-3)}$$

where:

$$\sigma_{\text{measure}} = \sqrt{\frac{\sum \left([SO_2]_{\text{measured}} - \overline{[SO_2]}_{\text{measured}} \right)^2}{N-1}}$$

All the SO_2 concentrations in Equation C-3 refer to the concentrations measured during the span checks. **Table C-6** shows the precision calculated for Bakersfield; the precision of the SO_2 measurements meets the CRPAQS DQO.

Table C-6. Precision and the number of span measurements used to calculate the precision of the 5-minute SO_2 data at Bakersfield.

No. of Spans Used	Absolute Precision at 40 ppb SO_2
65	0.2 ppb

6. REFERENCES

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